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Ferroelectric nanocomposites based on polymer ferroelectrics and graphene/oxide graphene: Computer modeling and SPFM experiments

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The experimental and computer modeling studies of composite nanomaterials based on polymer ferroelectrics polyvinylidene fluoride (PVDF)/poly(vinylidene fluoride-trifluoroethylene) (P(VDF-TrFE)) and graphene/oxide graphene (G/OG) are presented in this work. The main results of computer molecular modeling of the various nanostructures, piezoelectric properties of such combined nanocomposites of PVDF/(P(VDF-TrFE) thin films and G/GO layers were analysed in comparison with experimental data of the atomic force and scanning piezo-response force microscopy (AFM/SPFM). The computer simulation of the polymer-based nanocomposites of G/GO and PVDF was studied by the different methods using the HyperChem software package: molecular mechanics (MM), quantum mechanics (QM) using the semi-empirical PM3 and molecular dynamics (MD) runs. The piezoelectric response, the dielectric constant and the mechanical properties of the films were studied experimentally and found that they depend on the presence of the G/GO components concentration. The experimental results correlate qualitatively with the results obtained in these calculations. In particular, the calculated data of the piezoelectric coefficients d_{33} ~ 12 - 30 pm/C for PVDF-G/GO models corresponding to their observed experimental behavior, when the concentration of GO components are changed.

Then, using MD methods run with the quantum-chemical semi-empirical PM3 method, calculations of the change in the polarization with increasing temperature were carried out and a P(T) dependence was obtained. Data obtained was in agreement with the thermodynamic dependence of the polarization P(T), provided by Landau-Ginzburg-Devonshire theory for the ferroelectrics with a first-order phase transition (FP1). On the basis of this obtained relationship, the pyro-electric coefficients were calculated, which were in good agreement with the known values for the pure PVDF (~ 40 μC/(m^2*K)). For new nanocomposite models with graphene it turned out that in the case of a single-layer graphene model the pyroelectric coefficients increased by 3-4 times, and for the case of a two-layer model (sandwich model) it were decreased by 2-3 times in comparison with the pure polymeric ferroelectrics model. The experimental measurements of the pyroelectric coefficients values in these nanocomposites are in the work. The obtained results give important information about our understanding of the mechanisms of piezoelectricity and pyroelectricity in such nanocomposites, open new perspectives for the further creation, development and application of these new nanocomposites as multifunctional nanomaterials.

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